Modeling superconducting states of arbitrary pairing symmetry with the fluctuation exchange approximation applied to Hubbard-like models

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(Received 28 April 2009; revised manuscript received 23 July 2009; published 21 September 2009)

We present an algorithm for microscopic modeling of superconducting states of arbitrary pairing symmetry via an implementation of self-consistent perturbation theory, the fluctuation exchange approximation (FLEX), applied to Hubbard-like models. Like the original formulation of FLEX, all ring diagrams that are generated with the bare interaction vertex are included in the generating functional for the self-energy. Thus, this algorithm is suitable for FLEX-based Hubbard model calculations in both the attractive and repulsive cases.

DOI: 10.1103/PhysRevB.80.094516 PACS number(s): 71.10.Fd, 71.10.Li, 74.20.Mn, 74.20.Rp

I. INTRODUCTION

Since the emergence of Bardeen, Cooper, and Schrieffer's microscopic theory of superconductivity, analytic, and numerical modeling of electron pairing has played a central role in analysis of the processes by which superconductivity emerges in a wide variety of materials. While quantitative accuracy has been attained in the calculation of properties such as the superconducting transition temperature, T_c, for some materials, such as lead and aluminum, the lack of comparable success in modeling superconductors with strong electron correlations, such as the cuprates, leaves room for doubt as to the essential underlying physical processes responsible for superconductivity in those materials. However, theoretical arguments support the idea that, at least in principle, electron correlations can provide the pairing mechanism in addition to strongly renormalizing the normal state. Experiments as well as theoretical work have found that these strongly correlated superconductors are good candidates for having unconventional pairing states, i.e., where the spatial part of the wave function describing relative orientation of electron pairs is not of even symmetry with respect to the point-symmetry operations of the underlying lattice.[1]

For superconductors with strong correlations, a significant theoretical effort has focused on Hubbard-like Hamiltonians where the interactions between electrons are modeled with an effective repulsive or attractive atomic-ranged interaction,[2] an effort that was originally spurred by Anderson's hypothesis that the two-dimensional repulsive single-band Hubbard model provides a basic model for low-energy electronic properties in the cuprates.[3] The methods employed for this theoretical effort necessarily include some type of approximation that emphasizes a certain physical limit of the underlying, unsolved Hamiltonian.

The fluctuation exchange approximation (FLEX) developed by Bickers, Scalapino, and White[4] has attracted significant interest for model studies of the cuprates and other superconducting materials with strong correlations. As FLEX is based on self-consistent perturbation theory it is presumably most accurate in the limit of weak to moderate electron correlations. While the one-particle FLEX equations are derived systematically from a set of perturbation-theory diagrams for an underlying Hamiltonian, the equations produced nonetheless resemble those found in many spin-fluctuation models where the emergence of superconductivity is presumed to be driven by magnetic correlations. Consequently, it is not surprising that an unconventional, d-wave pairing state, is obtained using the FLEX treatment of the two-dimensional single-band Hubbard model near half filling,[5,6] as the same is observed in spin-fluctuation models with strong antiferromagnetic correlations and a similar band structure.[7] To the extent that spin fluctuations accurately describe the pairing mechanism in certain strongly correlated materials, the FLEX approximation applied to Hubbard-like models provides a viable modeling tool for these materials.

While the repulsive Hubbard model may provide a minimal model for the emergence of superconductivity in some strongly correlated systems, the attractive Hubbard model provides a conceptually simple model for superconductors with conventional pairing. In this case, an attractive electron interaction appears explicitly rather than emerging from a complex many-body process as must occur for superconductivity to emerge from a repulsive bare interaction. An advantageous feature of the attractive Hubbard model is its amenability to analysis via highly accurate quantum Monte Carlo techniques–accurate calculations for the two-dimensional attractive Hubbard model span over two decades.[8] It is indeed interesting that the Hubbard model may provide a tool for modeling both conventional and unconventional superconductors. Consequently, it is potentially useful for analysis schemes for the Hubbard model to work in both limits.

In this manuscript we present an algorithm for analysis of superconducting states with off-diagonal long-range order that is based on the application of FLEX to Hubbard-like models. To be clear, our interest here is in describing properties of systems below the transition temperature, T_c, where long-range off-diagonal order appears and thus go beyond Eliashberg-like schemes based on FLEX that aim to determine the dominant pairing symmetries and T_c through analysis of correlations in the normal state. The main features of our scheme are as follows. First, we incorporate s-wave particle-pair fluctuation terms; these are often neglected for the repulsive Hubbard model, leading to errors of up to 20% in the value of T_c,[5] but these terms are essential for the attractive Hubbard model and may play a role in determining the dominant pairing symmetry when one or more pairing state is favorable as may be the case with the pnictide

superconductors.[9,10] Second, we expand the pairing space to include triplet pairing, as may be observed in $SrRuO_4$ (Ref. 11) as well as mixed single-triplet pairing for lattices without inversion symmetry, like $CePt_3Si$,[12] or for systems with translational or magnetic disorder. Along with the generalizations necessary for nonsinglet pairing, the algorithm incorporates spin polarizations of arbitrary direction which is potentially useful for analyzing the competition and/or interdependence of competing magnetic and superconducting phases.

An important disadvantage of any FLEX-based calculation scheme is that FLEX is known to produce incorrect results in some limits. For example, *d*-wave pair fluctuations are not included in the approximation for the repulsive single-band Hubbard model so that a conventional broken symmetry state is produced at finite temperature in two dimensions,[5,6] a result that is in contradiction to general principles for two-dimensional phase transitions.[13,14] Also, the expected $T=0$ antiferromagnetically ordered state in two dimensions for the half-filled Hubbard model does not appear as expected.[15] These difficulties have been addressed in a variety of ways that may be well motivated on physical grounds, for instance by incorporating higher-order terms that are outside of the standard FLEX approximation, such as was done recently by Yan.[16] However, the many studies that have been performed using approximations based on FLEX have only added to the need for a clear presentation of a scheme for generalizing the FLEX approximation, as originally formulated, to states with long-range off-diagonal order and to the results that such a scheme produces.

II. ALGORITHM

For simplicity, we focus on a single-band Hubbard model, given by

$$H-\mu N=-\sum_{\langle \mathbf{r},\mathbf{r}'\rangle,\sigma} t(\mathbf{r}-\mathbf{r}')c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}\sigma}+\text{h.c.}-\mu\sum_{\mathbf{r},\sigma} c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}\sigma} - \sum_{\mathbf{r},\sigma,\sigma'} \mathbf{h}\cdot\vec{\sigma}_{\sigma\sigma'}c^{\dagger}_{\mathbf{r}\sigma}c_{\mathbf{r}\sigma'}+U\sum_{\mathbf{r}} c^{\dagger}_{\mathbf{r}\uparrow}c_{\mathbf{r}\uparrow}c^{\dagger}_{\mathbf{r}\downarrow}c_{\mathbf{r}\downarrow}. \quad (1)$$

where $t(\mathbf{r}-\mathbf{r}')$ describes the hopping between a pair of atomic sites at $\mathbf{r}$ and $\mathbf{r}'$, U is the on-site interaction amplitude between up and down spin electrons and $\mathbf{h}$ is the external magnetic field which we will assume here to be uniform through the lattice. We also include a pairing field term given by

$$H_p=\frac{1}{2}\sum_{\mathbf{r}\mathbf{r}'\sigma\sigma'} h_p(\Psi_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')c_{\mathbf{r}\sigma}c_{\mathbf{r}'\sigma'}+\Psi^{*}_{\sigma\sigma'}(\mathbf{r},\mathbf{r}')c^{\dagger}_{\mathbf{r}'\sigma'}c^{\dagger}_{\mathbf{r}\sigma}). \quad (2)$$

By monitoring the response of the system to a pairing field with a certain spatial and spin dependence given by $\Psi_{\sigma\sigma'}(\vec{r},\vec{r}')$ we can determine the superconducting correlations in that channel. In practice, we typically start with an exchange antisymmetric, but otherwise random form for Ψ and self-consistently determine the most dominant terms for Ψ. We note that such a static pairing field will not project states with odd-frequency pairing and, thus, such a procedure must be generalized to assess the relative stability of such states.[17] The external pairing field strength, h_p, governs the overall amplitude of the pairing field and can be reduced to zero to determine if a state with off-diagonal long-range order persists in the absence of such a field. To simplify the discussion, we will focus on a transitionally invariant superconducting states with zero-total momentum pairing channels such that $\Psi_{\sigma\sigma'}(\vec{r},\vec{r}')=\phi_{\sigma\sigma'}(\mathbf{r}-\mathbf{r}')$, although more general forms can be incorporated into this scheme. On each iteration we update ϕ according to

$$\langle c^{\dagger}_{\mathbf{r}'\sigma'}c^{\dagger}_{\mathbf{r}\sigma}\rangle=m_p\phi_{\sigma\sigma'}(\mathbf{r},\mathbf{r}'). \quad (3)$$

where ϕ is required to be normalized,

$$\sum_{\Delta\mathbf{r},\sigma,\sigma'} |\phi_{\sigma\sigma'}(\Delta\mathbf{r})|^2=1, \quad (4)$$

and the magnitude of m_p in Eq. (3) then provides a single number to characterize the strength of superconducting correlations in the system. Indeed m_p and h_p are analagous to the magnetization, m_z, and magnetic field, h_z, for a ferromagnetic transition.

After converting to momentum space, the noninteracting part of the Hamiltonian is then

$$H^{(0)}-\mu N=\sum_{\mathbf{k},\sigma}\xi(\mathbf{k})c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma}-\sum_{\mathbf{k}\sigma\sigma'}\mathbf{h}\cdot\vec{\sigma}_{\sigma\sigma'}c^{\dagger}_{\mathbf{k}\sigma}c_{\mathbf{k}\sigma'} - \frac{h_p}{2}\sum_{\mathbf{k},\sigma,\sigma'}(\phi_{\sigma\sigma'}(-\mathbf{k})c_{\mathbf{k}\sigma}c_{-\mathbf{k}\sigma'}+\phi^{*}_{\sigma'\sigma}(\mathbf{k})c^{\dagger}_{\mathbf{k}\sigma}c^{\dagger}_{-\mathbf{k}\sigma'}) \quad (5)$$

where $\xi(\mathbf{k})\equiv\epsilon(\mathbf{k})-\mu$ and $\epsilon(\mathbf{k})$ is the spatial Fourier transform of the hopping amplitude, $-t(\mathbf{r}-\mathbf{r}')$ and $\phi_{\sigma\sigma'}(\mathbf{k})$ is the same for the internal pair-wave function, $\phi_{\sigma\sigma'}(\mathbf{r})$.

We employ a Nambu representation to facilitate calculations in states with off-diagonal long-range order. In this representation we have a set of four annihilation operators

$$\{\psi_{\mathbf{k}0},\psi_{\mathbf{k}1},\psi_{\mathbf{k}2},\psi_{\mathbf{k}3}\}=\{c_{\mathbf{k}\uparrow},c_{\mathbf{k}\downarrow},c^{\dagger}_{-\mathbf{k}\uparrow},c^{\dagger}_{-\mathbf{k}\downarrow}\} \quad (6)$$

and likewise for creation operators. With the doubling of operator space, anomalous terms that appear with off-diagonal long-range order can be represented as a regular contraction of an annihilation and creation operator, i.e., $\langle c_{\mathbf{k}\uparrow}c_{-\mathbf{k}\downarrow}\rangle\equiv\langle\psi_{\mathbf{k}0}\psi^{\dagger}_{\mathbf{k}3}\rangle$. With this expansion of operator space, a physical process—such as the movement of an electron between sites—can be represented in more than one way and it will be important to ensure that these alternative representations of the same physical process are not overcounted when implementing an approximation such as FLEX.

The single-particle Green's function is defined as

$$G_{\alpha\alpha'}(\tau,\mathbf{k})\equiv-\mathcal{T}_{\tau}\langle\psi_{\mathbf{k}\alpha}(\tau)\psi^{\dagger}_{\mathbf{k}\alpha'}\rangle. \quad (7)$$

A matrix form for the noninteracting Green's function, $G^{(0)}$, is derived in the following manner. First, we use the standard result that

$$\frac{\partial \psi_{\mathbf{k}\alpha}(\tau)}{\partial \tau} = (\hat{H} - \mu\hat{N})\psi_{\mathbf{k}\alpha}(\tau) - \psi_{\mathbf{k}\alpha}(\tau)(\hat{H} - \mu\hat{N}) \tag{8}$$

$$= [(\hat{H} - \mu\hat{N}), \psi_{\mathbf{k}\alpha}(\tau)] \tag{9}$$

and perform the commutator algebra using the noninteracting part of the Hamiltonian to obtain a four-by-four set of linear equations for each $\mathbf{k}$ point, i.e.,

$$\frac{\partial \psi_{\mathbf{k}\alpha}(\tau)}{\partial \tau} = -\tilde{H}^{(0)}_{\alpha,\beta}(\mathbf{k})\psi_{\mathbf{k}\beta}(\tau) \tag{10}$$

where

$$\tilde{H}^{(0)}(\mathbf{k}) = \begin{pmatrix} \xi(\mathbf{k}) - h_z & -h_x + ih_y & h_p\phi^*_{\uparrow\uparrow}(-\mathbf{k}) & h_p\phi^*_{\uparrow\downarrow}(-\mathbf{k}) \\ -h_x - ih_y & \xi(\mathbf{k}) + h_z & h_p\phi^*_{\downarrow\uparrow}(-\mathbf{k}) & h_p\phi^*_{\downarrow\downarrow}(-\mathbf{k}) \\ h_p\phi_{\uparrow\uparrow}(-\mathbf{k}) & h_p\phi_{\downarrow\uparrow}(-\mathbf{k}) & -\xi(-\mathbf{k}) + h_z & h_x + ih_y \\ h_p\phi_{\uparrow\downarrow}(-\mathbf{k}) & h_p\phi_{\downarrow\downarrow}(-\mathbf{k}) & h_x - ih_y & -\xi(-\mathbf{k}) - h_z \end{pmatrix}. \tag{11}$$

The definition of the Green's function can be used to show that this set of equations also describes the time evolution of $G^{(0)}(\tau,\mathbf{k})$. This result is combined with the Fourier transform equation that produces the frequency domain representation of the Green's function, i.e.,

$$G(\varepsilon_n,\mathbf{k}) \equiv \int_0^\beta d\tau e^{i\varepsilon_n\tau} G(\tau,\mathbf{k}), \tag{12}$$

which after integration by parts yields

$$G(\varepsilon_n,\mathbf{k}) = \frac{1}{i\varepsilon_n}(G(\tau\to 0^-,\mathbf{k}) - G(\tau\to 0^+,\mathbf{k})) - \frac{1}{i\varepsilon_n}\int_0^\beta d\tau e^{i\varepsilon_n\tau}\frac{\partial G(\tau,\mathbf{k})}{\partial\tau}. \tag{13}$$

Upon substitution of the result from Eq. (10) into Eq. (13) as well as recognizing that $G(\tau\to 0^-,\mathbf{k}) - G(\tau\to 0^+,\mathbf{k})$ is equal to the identity matrix, a solution for the noninteracting Green's function is obtained having the form

$$G^{(0)}(\varepsilon_n,\mathbf{k}) = [i\varepsilon_n I - \tilde{H}^{(0)}(\mathbf{k})]^{-1}. \tag{14}$$

Interactions are incorporated into the Green's function via Dyson's equation and the self-energy, Σ,

$$G(\varepsilon_n,\mathbf{k}) = [(G^{(0)}(\varepsilon_n,\mathbf{k}))^{-1} - \Sigma(\varepsilon_n,\mathbf{k})]^{-1}. \tag{15}$$

In a phi-derivable conserving approximation such as FLEX, the self-energy is derived through a functional derivative,

$$\Sigma = \frac{\delta\Phi}{\delta G}, \tag{16}$$

where the generating functional, Φ, is approximated in terms of the Green's function and the bare interaction vertex. The symmetrized bare interaction vertex,[18] $\Gamma^{(0)}$, which is defined via

$$H_{int} = U\sum_{\mathbf{r}} c^\dagger_{\mathbf{r}\uparrow}c_{\mathbf{r}\uparrow}c^\dagger_{\mathbf{r}\downarrow}c_{\mathbf{r}\downarrow} \equiv \frac{1}{4!}\sum_{\mathbf{r},\alpha_1,\alpha_2,\alpha_3,\alpha_4}\Gamma^{(0)}_{\alpha_1\alpha_2;\alpha_3\alpha_4}\psi^\dagger_{\alpha_1}\psi^\dagger_{\alpha_2}\psi_{\alpha_4}\psi_{\alpha_3}, \tag{17}$$

has $4^4=256$ possible index combinations of which only 24 have the nonzero values of $+U$ or $-U$. The indices of the nonzero terms and their associated signs are $(01;01)=+$, $(01;10)=-$, $(03;03)=-$, $(03;30)=+$, $(02;13)=+$, $(02;31)=-$, $(10;10)=+$, $(10;01)=-$, $(12;12)=-$, $(12;21)=+$, $(13;02)=+$, $(13;20)=-$, $(23;23)=+$, $(23;32)=-$, $(21;21)=-$, $(21;12)=+$, $(20;31)=+$, $(20;13)=-$, $(32;32)=+$, $(32;23)=-$, $(30;30)=-$, $(30;03)=+$, $(31;20)=+$, and $(31;02)=-$. A graphical representation of this vertex function is given on the right of Fig. 1. In subsequent analysis, it will be convenient to have a representation for the bare vertex in terms of incoming and outgoing particle-hole pairs states rather than the representation of the vertex in terms of incoming and outgoing particle-particle pairs. Such a vertex, which will call $\Gamma^{(0)ph}$ is represented on the left side of Fig. 1. The relationship between the bare vertices in these two representations is given by

$$\Gamma^{(0)ph}_{\alpha_1\alpha_3;\alpha_4\alpha_2} \equiv \Gamma^{(0)}_{\alpha_1\alpha_2;\alpha_3\alpha_4}. \tag{18}$$

We will treat $\Gamma^{(0)ph}$ as a 16×16 matrix, effectively combining the first two indices into a single index for the outgoing

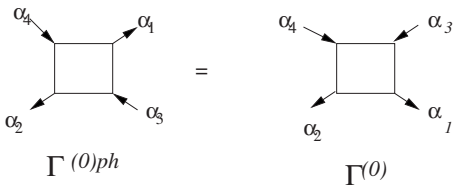

FIG. 1. Bare vertex function in the particle-hole representation, $\Gamma^{(0)ph}_{\alpha_1,\alpha_3;\alpha_4\alpha_2}$ and particle-particle representation $\Gamma^{(0)}_{\alpha_1,\alpha_2;\alpha_3\alpha_4}$.

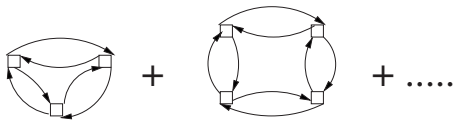

FIG. 2. Diagrammatic representation of third and fourth order particle-hole ring diagram contributions to Φ, the generating functional for the self-energy, Σ.

particle-hole configuration and the last two indices combining into a single index for the incoming particle-hole configuration.

In FLEX, contributions to Φ that are of second- and higher-order in terms of the interaction strength, U, are approximated through a set of ring diagrams. Particle-hole ring diagrams are represented diagrammatically in Fig. 2. In the original formulation of FLEX for the normal state, a set of particle-particle ring diagrams are added to the particle-hole diagrams to complete the graphical representation for the second- and higher-order terms. However, if all possible particle-hole diagrams within the expanded basis are included and the fully symmetrized bare vertex is properly defined, then the particle-particle ring diagrams in the formulation of FLEX for the normal state are already taken into account and, thus, this formalism restores this class of diagrams that are often neglected while using FLEX to model spin-fluctuation induced superconductivity via the repulsive Hubbard model. The penalty that is paid is that calculations involving the particle-hole terms have a large number of elements, owing to the larger number of initial and final particle-hole configurations in the expanded basis.

While evaluation of Φ itself is needed to obtain results for various thermodynamic quantities such as the entropy, we will limit ourselves to providing the necessary expressions for calculating the self-energy which is the most computationally intensive part of the iterative FLEX equations. After an expression for Φ is constructed according to diagrammatic rules, including symmetry factors that are needed because of the use of our expanded basis, and taking the functional derivative to obtain the electron self-energy, we obtain

$$\Sigma^{n\geq 2}_{\alpha\alpha'}(\tau,\mathbf{r}) = -\sum_{\alpha_1\alpha_2} G_{\alpha_1\alpha_2}(\tau,\mathbf{r})\tilde{T}_{\alpha\alpha_2;\alpha'\alpha_2}(\tau,\mathbf{r}) \tag{19}$$

where the particle-hole t-matrix, $\tilde{T}$, is given in frequency and momentum space by

$$\tilde{T}(\omega_n,\mathbf{q}) = \left[\frac{\tilde{\chi}(\omega_n,\mathbf{q})}{2} + [\tilde{\chi}(\omega_n,\mathbf{q})]^2[I-\tilde{\chi}(\mathbf{q},\omega_n)]^{-1}\right]\Gamma^{(0)ph} \tag{20}$$

with

$$\tilde{\chi}(\tau,\mathbf{r}) = -\frac{1}{2}\Gamma^{(0)ph}\chi(\tau,\mathbf{r}) \tag{21}$$

and

$$\chi_{\alpha_1\alpha_2;\alpha_3\alpha_4}(\tau,\mathbf{r}) \equiv (-1)G_{\alpha_1\alpha_3}(\tau,\mathbf{r})G_{\alpha_4\alpha_2}(-\tau,-\mathbf{r}). \tag{22}$$

In Eqs. (20) and (21), it is understood that for every unique set of frequency/momentum or time/space values the quantities that appear in the equations are 16×16 matrices.

For completeness, we also note the first-order contribution to the self-energy. For a transitionally invariant system we have

$$\Sigma^{n=1}_{\alpha\alpha'}(\tau,\mathbf{r}) = \sum_{\alpha_1,\alpha_2}\Gamma^{(0)}_{\alpha_1\alpha;\alpha_2\alpha'}G_{\alpha_2\alpha_1}(\tau=0,\mathbf{r}=\mathbf{0})\delta_{\mathbf{r},\mathbf{0}}\delta(\tau). \tag{23}$$

The $\tau\to 0$ limit for Σ is ambiguous for $\alpha=\alpha'$ and for G when $\alpha_2=\alpha_1$ in the sum. In such instances the appropriate limits are $\tau\to 0^-$ for $\alpha=0$ or 1 and $\tau\to 0^+$ for $\alpha=2$ or 3.

We follow Serene and Hess in using Fourier transform techniques to reduce the scaling of the FLEX calculations to order $N\ln N$ where N is the number of unique space/time points in the calculation.[19] We use the method of Deisz, Hess, and Serene to improve the numerical accuracy of the finite representation of the time/frequency domain;[20] the resulting errors are well-controlled and are not discussed further here. We employ the dynamical cluster approximation (DCA) to accelerate the convergence of results as a function of lattice size.[21,22] In this formalism, a many-body calculation (using FLEX in this case) for an $N_l=L_x\times L_y\times L_z$ lattice is simplified through the use of an $N_c=L_{cx}\times L_{cy}\times L_{cz}\leq N_l$ effective dynamical cluster for estimating correlation effects. We will note values of N_c used in our calculations, but it will not be the purpose of this manuscript to explore convergence with N_c in detail.

III. DEMONSTRATIONS

A. *d*-wave superconductivity in the two-dimensional repulsive Hubbard model

The fluctuation exchange approximation applied to the single-band Hubbard model near half-filling has been used extensively for modeling d-wave superconductivity in the cuprates. Some of this work is based on analysis of pairing instabilities in the normal state,[23] a procedure that yields transition temperatures, T_c, as well as the symmetry group that provides the basis for the pair-wave function. Other work includes explicit calculation and analysis below T_c,[5,6] encompassing the properties extracted from the instability analysis and other properties such as the temperature dependence of the superconducting gap function.

In the top half of Fig. 3 we show a graph of FLEX results obtained with this algorithm for the pairing amplitude, m_p, versus temperature for a density of $n=0.85$ electrons per site, $U/t=4.0$ where t is the nearest-neighbor hopping amplitude, i.e., $t=t(\Delta x\hat{x})$ and Δx is the spacing between lattice points in the x direction (all other hopping amplitudes are set equal to zero in this case) and using a $N_c=16^2$ DCA cluster with an underlying $N_l=64^2$ lattice. A fit (dashed line) to the numerical results (open circles) provides an estimate of T_c. Performing similar calculations for a range of parameters produces a section of the phase diagram as shown in the bottom of Fig.

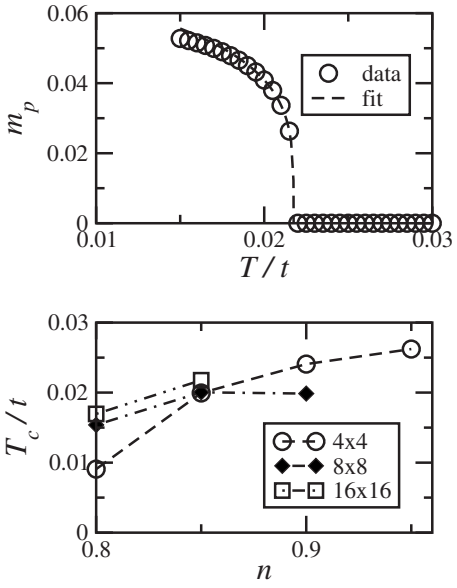

FIG. 3. (Top) Pairing amplitude, m_p, vs scaled temperature, T/t, for the repulsive Hubbard model with $U=4t$, a density of 0.85 electrons per site and t is the nearest-neighbor-hopping amplitude in the limit that $h_p \rightarrow 0$. Calculation was performed with a 16×16 dynamical cluster embedded in a 64×64 lattice using the dynamical cluster approximation. A fit (dashed line) to the FLEX data (circles) is used to estimate the transition temperature T_c. (Bottom) Scaled superconducting transition temperature, T_c, versus electron density per atomic site, n. All calculations were performed with $U=4t$ and an underlying 64×64 lattice. The results are consistent with those produced by Pao and Bickers by analyzing pairing instabilities in the normal state. Some variation is observed with respect to cluster size in going from 4×4 to 16×16 clusters. Results for large clusters and densities near $n=1.0$ are difficult to obtain on account of singular features in FLEX calculations that make convergence slow at low temperatures.

3. These results track well what has been obtained in previously reported FLEX calculations for the same model parameters. For example, as noted by Pao and Bickers,[5] the pairing amplitude does not have the mean-field form $m_p \sim (T_c - T)^{1/2}$ as in our case the exponent is closer to 0.2. Our best estimate for T_c for $n=0.85$, $T_c/t \simeq 0.022$ agrees well with that obtained by Bickers and White[23] from an instability analysis. Finally, the T_c vs n trends concur with that obtained by Pao and Bickers for $U=6t$.[24]

Figure 3 also reveals a weakness in our approach in that as the DCA cluster size gets larger it becomes increasingly difficult for the FLEX equations to converge at low temperatures in the vicinity of $n=1.0$ on account of numerical instabilities assosciated with singularities in the t matrix that are due to (nearly) perfect nesting of the Fermi surface. This convergence problem is less severe in an instability analysis as the calculations in that case are done for higher temperature values, namely, $T > T_c$. This limitation of the algorithm does not persist when a next-nearest-neighbor hopping term is included in the Hamiltonian as is frequently done for this model.

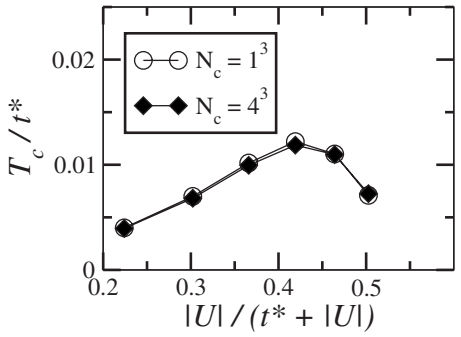

FIG. 4. Scaled superconducting transition temperature, T_c/t^*, versus scaled interaction strength, $|U|/(t^*+|U|)$, for the three-dimensional attractive Hubbard model with a density of one-electron per site where $t^*=2\sqrt{d}t \simeq 2.8t$ is a measure of the electron bandwidth as a function of spatial dimension d. Calculations were performed using an $N_L=16^3$ lattice, but with correlations evaluated using $N_c=1^3$ (open circles) and $N_c=4^3$ (filled diamonds) clusters as prescribed by the dynamical cluster approximation. The weak dependence of T_c/t^* results as a function of N_c demonstrate the smallness of corrections to dynamical mean-field theory, which becomes exact in the infinite dimensional limit, at least for the parameters and approximation scheme explored here. These results are in excellent agreement with those obtained by Freericks in the infinite dimensional limit. (Ref. 25)

B. Superconductivity in the attractive Hubbard model

The Hubbard Hamiltonian with an attractive interaction between up and down spin electrons provides a simple model for even spatial symmetry (s wave) electron pairing. Freericks explored the accuracy of FLEX by considering the infinite dimensional limit of the Hubbard Hamiltonian where dynamical correlations between electrons become purely local,[25] greatly simplifying the analysis whether it is done through quantum Monte Carlo or through an approximation scheme such as FLEX.[26] Freericks explicitly focused on the charge-density wave transition that occurs in the model at half filling, but this transition is degenerate with an s-wave superconducting transition and, thus, his results provide a test for this algorithm.

Following Freericks, in Fig. 4 we display results for the transition scaled transition temperature, T_c/t^*, versus the scaled interaction strength $|U|/(t^*+|U|)$ where $t^* \equiv (2\sqrt{d})t$ is a measure of the electron bandwidth as a function of lattice dimension, d. We use the DCA to approximate correlations using cluster sizes of $N_c=1^3$ and $N_c=4^3$ and find little dependence of these results on N_c, thus validating the use of dynamical mean-field theory, i.e., $N_c=1^3$, for the model parameters considered here. Indeed the details of this graph are in excellent agreement with Freericks' results for the $d \rightarrow \infty$ limit, including both the location and size of the maximum in T_c/t^*.

C. Search for p-wave superconductivity in the repulsive Hubbard model at low particle density

In the limit of low density, the Hubbard model with a repulsive interaction has a tendency to produce ferromagnetic correlations. In turn, these correlations may drive a su-

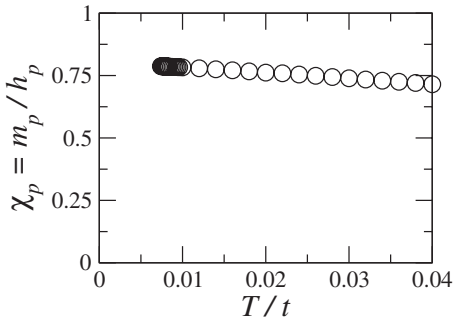

FIG. 5. Pairing susceptibility, χ_p, in the p-wave channel for the one-band repulsive Hubbard model at $n=0.3$ electrons per site, $U=4t$ and a nearest-neighbor-hopping term $t'=-0.5t$. Although ferromagnetic correlations are strong, no transition to a p-wave superconducting state is observed as the temperature is lowered, in concurrence with previous results based on an instability analysis.

perconducting transition to a state with spin-triplet orbital p-wave pairing. While there is extensive theoretical work with respect to this possibility, we will focus on the FLEX results of Arita, Kurok, and Aoki[27] as a point of comparison for our implementation of this approximation.

In their work, they include a next-nearest-neighbor hopping term, t', i.e., $t'=t(\Delta x\hat{x}+\Delta y\hat{y})$, to enhance the ferromagnetic correlations that are needed to produce p-wave pairing within FLEX. Quantum Monte Carlo simulations suggest an optimal value of approximately $t'=-0.5t$ for an electron density of 0.3 per atomic site.[28] Their analysis of pairing instabilities in the normal state nonetheless does not reveal a strong tendency toward a p-wave pairing state, at least down to the fairly small temperatures, $T/t\sim 0.02$, considered in their study.

This approach, in which we apply a small pairing field, h_p, and then monitor the resulting pairing response, m_p, for instabilities, differs technically from that of Arita, Kuroki, and Aoki, but should, in principle, produce the same qualitative results, although some quantitative differences are expected as particle-particle contributions to the electron self-energy and pairing vertices were neglected in the instability analysis. Indeed, as shown in Fig. 5 our pairing susceptibility, $\chi_p\sim m_p/h_p$ with h_p small (namely, $h_p\sim 0.001t$; smaller values for h_p do not change this ratio), is essentially flat to the lowest temperatures for which we are able to obtain converged results, $T/t\sim 0.01$, in concurrence with the instability analysis results. While we do not have a diverging pairing response as temperature is lowered, we have verified that the dominant pairing symmetry that emerges from our analysis is p wave.

IV. SUMMARY AND FUTURE DIRECTIONS

We presented an algorithm for FLEX calculations for superconducting states of arbitrary pairing symmetry and have demonstrated its ability to reproduce previously obtained results for s-wave superconductivity in the attractive Hubbard model and d- and p-wave superconductivity in the repulsive Hubbard model. On account of the generality of the algorithm, it provides a framework for FLEX studies of superconductivity in systems with nonsinglet pairing and systems where there is more than one strong candidate for the pairing symmetry.

Extensions to the multiband models, such as would be appropriate for the pnictide superconductors, simply follow by expanding the local operator space in the Nambu representation from four components to $4N_b$ components where N_b is the number of bands in the model. However, the particle-hole such as quantities χ, $\tilde{\chi}$, and $\tilde{T}$ that are computed on very iteration of FLEX scale have $(4N_b)^4$ components for each time/space or frequency/momentum value. Thus, a five-band model would lead to at least a $5^4=625$ factor increase in storage and calculation of these quantities. Such a calculation is feasible, particularly if the dynamical cluster approximation is use to reduce the effective spatial scale that is needed to perform the parts of the calculation where these quantities appear. While FLEX calculations of normal-state instabilities have already been performed, they point to the possibility that more that while a type of s-wave pairing symmetry is strongest, electron correlations make other types of pairing feasible as well.[9,10] This being the case, it is especially important to perform investigations below T_c as a second superconducting transition my occur below T_c, as is observed in FLEX calculation of the repulsive three-dimensional Hubbard model with tetragonal, but nearly cubic symmetry.[29]

ACKNOWLEDGMENTS

J.J.D. gratefully acknowledges partial support from the Graduate College of the University of Northern Iowa. T.J.S. gratefully acknowledges partial support from the College of Natural Sciences of the University of Northern Iowa.

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